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Supplementary material. Listings of the restraints and the achieved distances from molecular modeling of the (2-PyN)$_2$-C6·5'-TGACT-3' complex[a]

Intermolecular ligand-DNA restraints:

Peptide 1	DNA	Peptide 2	Restraint in Å	Distance in Å
	A19 C1'H	NH-3	2.5-3.7	3.79
	A19 C1'H	H3-3	2.5-3.7	3.25
H6	G5 C1'H		2.5-3.7	2.78
H6	G5 NH_2[b]		1.8-5.0	3.81
	C18 C1'H	NH-2	1.8-2.5	2.58
	C18 C1'H	H3-2	1.8-3.7	3.06
NH-1	A6 C1'H		2.5-3.7	2.85
NH-1	A6 C2H		2.5-3.7	3.06
H3-2	A6 C2H		1.8-2.5	2.51
NH-2	A6 C2H		2.5-3.7	3.72
	A6 C2H	H3-2	1.8-3.7	2.88
	A6 C2H	NH-1	2.5-3.7	3.80
	T17 C1'H	NH-1	1.8-2.5	2.57
H3-2	C7 C1'H		1.8-2.5	2.56
NH-2	C7 C1'H		1.8-2.5	2.41
	G16 C1'H	H6	2.5-3.7	2.47
	G16 NH_2[b]	H6	1.8-5.0	3.72
H3-3	T8 C1'H		2.5-3.7	3.31
NH-3	T8 C1'H		2.5-3.7	3.74

Intramolecular ligand restraints:

Peptide 1		Restraint in Å	Distance in Å
NH-1 to	H3-2	2.5-3.7	2.57
H3-2 to	NH-2	1.8-2.5	2.16
NH-2 to	H3-3	2.5-3.7	2.57
H3-3 to	NH-3	1.8-2.5	2.11
Peptide 2		**Restraint in Å**	**Distance in Å**
NH-1 to	H3-2	2.5-3.7	2.64
H3-2 to	NH-2	1.8-3.7	2.40
NH-2 to	H3-3	2.5-3.7	2.65
H3-3 to	NH-3	1.8-2.5	2.14

[a]Restraints for the hydrogen bonds in the Watson-Crick base pairs were 1.65 - 2.05 Å.

[b]Restraint to the nitrogen atom of the guanine amino group.